UDC 666.1.022(083.1):66.012-52

AUTOMATION OF BATCH FORMULA CALCULATION

M. M. Khaimovich[1] and K. Yu. Subbotin[1]

Translated from Steklo i Keramika, No. 4, pp. 27 – 30, April, 2005.

Problems arising in automating the calculation of the glass batch formula and algorithms used to solve this problem are considered. A universal programs for automating the batch formula calculation is described.

The calculation of a batch formula is a significant target of chemical laboratories at glass and other factories that have to melt batch to produce finished products (for instance, electromelted refractory works, frit-producing divisions at metallurgical and ceramic works).

Errors in formula calculation are hard to identify and yet they can have a perceptible effect on the finished product quality. Mass-scale defects of finished products, if they are related to calculation errors, are usually attributed to the quality of batch proportioning and mixing or to the violation of the technological regime of the furnace.

Setting the problem of calculating batch formulas and methods for solving this problem by manual calculations are extensively described in the literature [1 – 4]. The weight content of oxides in glass and in components is specified in percent. Thereupon one obtains a system of linear equations, in which the unknown is the quantity of each component needed to produce 100 kg of glass. Each equation is determined by an oxide specified in the formula. In a correct setting of the problem the number of linear-independent equations and the unknowns ought to coincide.

However, laboratories at different companies use different approaches to specifying the set of oxides and materials and to the setting of a system of equations and, accordingly, to calculation details. These specifics should be analyzed in detail.

The analysis of the chemical composition of soda, sulfate, and feldspar usually identifies their weight content of Na_2O, Na_2CO_3, Na_2SO_4, K_2O, K_2CO_3, and K_2SO_4, whereas the only component specified for the glass composition is the content of Na_2O. Therefore, before starting the main calculation of the batch formula, its components are converted using the coefficient of their atomic weights ratio, taking into account the fact that CO_2 evaporates in glass melting and the content of SO_3 in glass is accounted for separately.

Moreover, both soda and sulfate introduce into glass only alkalis (Na_2O), therefore, without additional data it is impossible to determine the quantity of both materials, since both variables are contained only in one equation, and, consequently, the number of solutions in this case is infinite. To solve this contradiction, most laboratories use a parameter called “the percent of alkalis introduced via sulfate.” At different factories this percent is understood in different ways: either as the content of Na_2O in glass introduced via sulfate, or as percent (fraction) of the total content of Na_2O in glass. At the same time, laboratories usually specify the content of SO_3 in the glass formula, thus ignoring the doubling of the information, since in determining the percent of alkalis introduced via sulfate, the content of SO_3 determines the quantity of sulfate (this yields an additional equation for sulfate and separates it from soda). On the other hand, setting the percent of alkalis introduced via sulfate uniquely determines the content of SO_3 that will be contained in glass.

Chemists performing the formula calculation can rarely explain why the content of Fe_2O_3 and Al_2O_3 in the composition of components is specified separately, whereas the glass formula specifies a combined percent of R_2O_3 (sesquioxides). Such procedure is applied at factories that do not use iron oxide or crocus. If the oxides are not combined in the glass formula, the number of equations is fewer than the number of unknown quantities and the system has no solution. However, since each of the oxides is responsible for different properties of glass, it is advisable to perform calculations based only on Al_2O_3 (in other words, specify Al_2O_3 in the glass formula rather than R_2O_3), whereas Fe_2O_3 will be determined based on its actual content in the components. Similarly, in those cases where carbonates are introduced into the batch only via dolomite (without chalk or lime) and the glass formula specifies RO combining CaO and MgO, it is advisable to calculate the carbonates only based on CaO (i.e., to specify CaO in the glass formula rather than RO), whereas MgO will be determined based on its content in dolomite.

The account of entrainment percent (sometimes aspiration percent) is complicated by the fact that different labora-

[1] Stromizmeritel’ Joint-Stock Company, Nizhny Novgorod, Russia.

tories regard and determine this percent in different ways. Some of them only calculate losses in transporting materials and batches from the weighing proportioners to the furnace loaders. Others take into account volatilization inside the furnace. Norms on these values are vague and usually based on practical experience.

The quantity of water supplied for batch mixing is usually adjusted several times per shift based on the batch moisture data provided by the current laboratory analysis and not specified in the formula calculation. However, some factories perform such a calculation. This is due to the fact that the moisture of a batch fed into a furnace depends not only on the moisture of its components, but also on moisture losses in transportation and storage and the moisture of added cullet, which may vary (especially in imported cullet) depending on particular deliveries or even on the weather. However, it should be noted that virtually all attempts to calculate the quantity of water required to obtain a batch of a certain moisture yield insufficient quantities. This is probably due to the reaction between water and the batch components (in particular, soda).

The above is also true of the calculation of the amount of added cullet, which is usually specified in percent of the mixture of batch and cullet. However, different interpretations are found. Most often the batch : cullet ratio is specified as the ratio of the batch weight without water but accounting for the moisture of batch materials and the weight of the cullet taking into account its moisture. This is convenient for calculating the amount of cullet that has to be proportioned using a discrete dosing weigher. In using a continuous proportioner [5] the content of the cullet has to be specified in proportion to the weight of the batch taking into account added water, since this is the batch that is weighed when passing through the weighing gages of the conveyor belt. Some factories specify the batch : cullet ratio based on the quantity of the resulting glass melt. In this case to determine the quantity of cullet (when weighed by a discrete dosing unit) or its percent (when dosing by a continuous proportioner), one should take into account the burning loss of the batch (percent) in addition to its moisture.

Some factories using large quantities of imported cullet set the additional target of calculating the oxide composition of the cullet for calculating the batch formula. However, this approach appears questionable, since it is difficult to get an averaged estimate of the composition of imported glass cullet with an acceptable accuracy.

The burning loss as well is calculated in different ways. Most factories calculate burning losses based on dry batch ignoring entrainment; however, for some factories it is significant to calculate burning losses with entrainment, and some factories in calculating burning loss take into account moisture as well, not only the moisture of the components but added water as well.

In manual calculations these specifics usually remain unnoticed, since they become habitual and are regarded as “unchangeable.” However, in developing automated programs for batch formulas they have to be taken into account, otherwise the implementation of a computerized program will cause serious difficulties to the manufacturer.

Programs for automatic calculation of the batch formulas are usually developed on the basis of a particular factory taking into account the specifics of only this factory. Most programs are written in Microsoft Excel and lack the necessary flexibility, since in introducing new components or changing to new glass compositions good knowledge of this application is required of the user.

The calculation methods used in the automatic program for glass batch calculation developed by the Stromizmeritel’ JSC have been determined by the problem setting. To solve a system of linear equations, mathematicians use the method of elimination of variables (the Gauss method) and the Gauss – Zeidel iteration method [6] providing an exact solution to systems in which the number of unknowns is equal to the number of linear-dependent equations. If this condition is not satisfied, the results depend on which number is larger.

If the number of components in a batch formula is larger than the number of oxides remaining in the calculation after preliminary processing (which includes converting the oxides from materials that are not found in the formula to oxides in the formula and taking into account the preliminary calculation formulas), the desired quantity cannot be calculated for one or several components (the system of equations has an infinite number of solutions); consequently, some oxides should be added to the formula, or some materials excluded from it.

In the case of a disagreement between the number of materials and the number of oxides, various methods are proposed for approximate solutions (the least square method, the V-problem of linear programming, etc.) [4, 6]. These methods optimize the total deviations for all oxides. For practical chemists the result obtained by the Gauss – Zeidel method is more acceptable and understandable. In this case in manual calculations the situation of a disagreement between the number of materials and the number of oxides is resolved automatically. If the number of materials is larger, this means that several materials have to be calculated based on the same oxide (for instance sulfate and soda based on Na_2O). In this case an additional condition is imposed (percent of alkalis introduced via sulfate) and one of the materials is excluded from the equation system at the preliminary stage. If the number of oxides is larger, some oxides are simply not included in the calculation, since each material is calculated based on a certain oxide. For oxides not used in the calculation (for instance Fe_2O_3 and SO_3) their percent in glass is calculated after determining the quantity of the components per 100 kg of glass.

The proposed program takes into account this practice. If the number of components making up a system of equations is larger than the number of oxides, the program issues the message: “Material ... is irresolvable” and sets the quantity of this material equal to zero. If the number of oxides is larger, the program gives a nonzero error in the result for the

oxides that are not used. By counting the oxides with a nonzero error, we know by how many the number of oxides in the formula exceeds the number of materials. The oxides with a nonzero error are those whose weight content in the formula is low, which is determined by the algorithm.

The program uses the Gauss method for solving the problem, which is preferable for programming, faster in performance, and yields better accuracy.

The manual calculation of the batch formula performed by laboratories using a manual calculator usually provides a satisfactory accuracy. However, in some cases problems arise that lead to significant errors in formula calculations. If the computation with a calculator take into account only two digits after the integer number, the error can reach 0.5%. If the procedure does not specify the need to repeat the computations at least three times, the calculation error reaches 1%.

Most factories in manual calculations take into account four digits after the integer number and perform three iterations according to the Gauss – Zeidel method. In this case the accuracy of the results with respect to the deviation of oxide content from the quantity specified in the formula is not more than 0.2%. Computer modeling of calculations based on the Gauss – Zeidel method indicates that after three iterations the accuracy is around 0.1%. To obtain an accuracy better than 0.0001% the number of iterations has to be at least eight.

The above-mentioned errors in manual calculations have led to an incorrect estimate of the performance of proportioning equipment and, accordingly, problems have arisen during the acceptance of batch-proportioning and mixing divisions, Therefore, we have added an inverse calculation module in the programs for the automatic batch calculation for determining the content of oxides in glass based on the quantity of components per 100 kg of glass. This makes it possible to estimate the accuracy of the calculations, both manual and automatic. Such estimate corroborates the fact that even with significant differences in the results of manual and automated calculations (for some components the difference may reach a few kilograms), the error in the glass composition does not exceed 0.1 – 0.2% for all oxides. This suggests that the problem is resistant to balance deviations in proportioning specifications related to calculation errors.

The program for automatic calculation of batch formulas developed by Stromizmeritel' JSC takes into account all the above and provides a universal approach to the calculation of formulas. However, the universality has another aspect, which leads to certain difficulties in its implementation. To develop a new formula in the case of replacing certain materials or modifying their oxide content, the program has a tuning module. However, preparatory tunings are not frequent.

When the tuning has been performed, the user sees on the display window the following data that are customary for manual calculations:

– the table for specifying the weight content of oxides in components expressed in percent, with additional columns for specifying the price per kilo, the entrainment percent, and the moisture of each component;

– the table with a preset content of oxides in glass, in percent;

– fields for specifying the required batch moisture and the amount of a portion to be mixed (melted);

– additional field for specifying the amount of alkalis introduced via sulfate or adding cullet (in percent) if they are specified during the tuning of the formula.

The universality of the program makes it possible to calculate a prescribed batch quantity (for continuous furnaces) or a portion to be melted (for batch furnaces, for instance, in the production of electromelted refractories).

It should be noted that in the table for specifying components indicating oxides contained in them one can enter oxides not indicated in the table of the glass composition. If these oxides in tuning are related to the oxides specified in the glass composition, the conversion is performed automatically, in accordance with the tuning-specified coefficient. For instance, if the table of components lists Na_2CO_3 and Na_2SO_4, while the formula table has only Na_2O and at the same time the tuning specifies the coefficient of conversion of Na_2CO_3 into Na_2O equal to 0.5848 and the conversion coefficient of Na_2SO_4 into Na_2O equal to 0.4363, then before the start of the calculation the percent of Na_2CO_3 in the material will be multiplied by 0.5848, Na_2SO_4 multiplied by 0.4363, summed, and added to the Na_2O percent in the materials. The latter value will be used in the calculation.

After the tables of initial data are filled, the operator presses the button "calculation of formula," starts the calculation, and the window of calculated results is opened. This window has three tables.

The first table is customary for chemists and specifies the percent of each oxide introduced per 100 kg of glass melt by each batch component; the amount of material per 100 kg of glass melt with and without entrainment; the amount of material per 100 kg of batch and per batch portion with and without account of moisture. The bottom line specifies the quantity of each oxide per 100 kg of glass as the sum of all components. It should be noted the oxides in this table are taken from the table specifying the percent of materials, i.e., if the content of Fe_2O_3 and Al_2O_3 in the material is specified separately and the glass specifies a combined percent of sequioxides, the values in this tables will be calculated separately.

If the specification of components includes an oxide that is not present in the prescribed glass composition and cannot be reduced to any of the oxides in the glass composition, a warning will be issued in the course of the calculation, but the final table will specify the quantity of this oxide introduced by individual materials and its total content in the glass composition. This provides an estimate of the quantity of oxides for which control values are not specified and calculations are not carried out.

The second table displayed is intended to estimate the deviation of the calculation results from the prescribed glass composition. This table for each oxide included in the glass composition specifies the following data: initially set value, total value for 100 kg of glass and their difference determining the deviation of the calculated value from the preset value. If the content of Fe_2O_3 and Al_2O_3 in materials is set separately and the glass formula gives a combined percent of sequioxides R_2O_3, the table indicates the values for R_2O_3. If the quantity of oxides in the glass formula is larger than the quantity of materials and the system has no exact solution, the table will make it possible to estimate the deviation of the calculated glass composition from the preset composition.

The third table indicates the burning loss values and the expected results of the chemical analysis of the batch (theoretical composition) without entrainment and moisture, with account of only entrainment, and with account of entrainment and moisture.

The proposed program allows for getting a printout of initial data and calculation results, printout of the proportioning task, and storing results for a subsequent review.

The program for automated batch formula calculation has been developed for the purpose of computerizing the work of chemical laboratories at industrial enterprises and was initially supplied together with automated control systems for proportioning and mixing divisions. The program was based on the requirements of the central factory laboratory at the Kavminsteklo JSC.

The programs has been implemented at more than 20 glass factories and approved by their chemical laboratories. The program is being constantly upgraded in accordance with new requirements imposed by users. The tuning possibilities provide for the batch formula calculation for electromelted refractories (it is successfully applied at the Shcherbinskii and Domodedovskii electromelted refractory works). The implementation of this program in the experimental laboratory of LMZ-Stema Lys'venskii Metallurgical Works has demonstrated the possibility of the automated calculation of batch formulas for frit production.

The next phase of this program will be the automation of the chemist's working place with automated transfer of the proportioning task to the automated control system of the dosing and mixing division.

REFERENCES

1. V. M. Budov and P. D. Sarkisov, *Production of Construction and Technical Glass* [in Russian], Vysshaya Shkola, Moscow (1985).
2. V. I. Panasyuk, *Chemical Analysis of Glass and Raw Materials* [in Russian], Stroiizdat, Moscow (1971).
3. N. A. Yudin and A. I. Zaporozhskii, *Technology of Glass Containers and Household Glass* [in Russian], Vysshaya Shkola, Moscow (1989).
4. E. P. Markov, A. G. Chesnokov, V. E. Manevich, and A. I. Ovcharenko, "Analysis of methods for calculation of glass batch," *Steklo Keram.*, No. 12, 3 – 4 (1980).
5. V. V. Efremenkov, K. Yu. Subbotin, and M. M. Khaimovich, "A system for proportioning batch and cullet into glass-melting furnace," *Steklo Keram.*, No. 6, 3 – 4 (2001).
6. B. P. Demidovich and I. A. Maron, *Principles of Computational Mathematics* [in Russian], Nauka, Moscow (1966).